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SENSITIVITY ANALYSIS OF INITIAL VALUE PROBLEMS WITH MIXED ODE'S AND ALGEBRAIC EQUATIONS

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ABSTRACT

An efficient method is described for sensitivity analysis of nonlinear initial value problems, which may include algebraic equations as well as ordinary differential equations (ODE's).

The linearity of the sensitivity equations is utilized to solve them directly via the local Jacobian of the state equations. The method is implemented with the implicit integrator DASSL and is demonstrated on a stiff industrial reaction model.

AMS (MOS) Subject Classifications: 34-04, 65L05, 65H10

Key Words: Numerical integration, Stiff equations, Parametric sensitivities, Initial value problems, Newton's method, Chemical kinetics.

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SIGNIFICANCE AND EXPLANATION

Many physical systems are modelled by systems of ordinary differential and algebraic equations with initial conditions. The solution vector $\underline{u}$ depends on the time t, and on a vector $\underline{\theta}$ of unknown parameters. This report deals with the calculation of the first-order parametric sensitivities, $W_{ik}(t,\underline{\theta}) = \partial u_i/\partial \theta_k$, which are useful in parameter estimation, system design and control.

The method given here takes advantage of the similarity of the backward difference forms of the u-equations and W-equations, as well as the linearity of the W-equations, to achieve unusually fast solutions with minimal memory requirements. The method has been implemented as a modification of the program package DASSL. Numerical results are given for a chemical kinetic example.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the authors of this report.

SCOPE

With the rapid development of digital computers, increasingly realistic mathematical models are being used to investigate chemical phenomena. New mechanistic features, however, call for new physicochemical parameters whose values may not be accurately known. Consequently, there is an increasing need for parametric sensitivity analysis of proposed differential and algebraic models.

Parametric sensitivity analysis is a very active research area. Extensive reviews can be found in Rabitz et al. [14], and in Tilden et al. [17]. Applications occur in every engineering and scientific discipline. Potential areas of application in chemical engineering include optimization, parameter estimation, model simplification, process sensitivity and multiplicity, experimental design and many more.

In this paper we address the problem of numerical computation of sensitivity functions for systems of ordinary differential and algebraic equations. We develop a simple, efficient algorithm for this purpose by extension of a standard implicit integrator.

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PROBLEM STATEMENT.

Consider a dynamic system, described by the following set of differential and algebraic equations:

$$\underline{E}\underline{u}'(t) = \underline{f}(t,\underline{u}(t);\underline{\theta}) \tag{1a}$$

$$\underline{u}(t=t_0) = \underline{u}_0(\underline{\theta}) \tag{1b}$$

Here $\underline{u}$ is an n-dimensional vector of state variables, $\underline{\theta}$ is an m-dimensional vector of time-independent parameters and $\underline{E}$ is an (n,n) matrix of constant coefficients. Most frequently in chemical kinetics calculations the matrix $\underline{E}$ assumes the form

$$\underline{E} = \begin{bmatrix} \underline{I}^{(s)} & \vdots & \underline{0} \\ \cdots & \vdots & \cdots \\ \underline{0} & \vdots & \underline{0} \end{bmatrix} \tag{2}$$

where $\underline{I}^{(s)}$ is the identity matrix of order s. If s = n, system (1a) consists of purely differential equations. If $1 < s < n$, system (1a) consists of ordinary differential and algebraic equations. The latter case arises, for instance, in analysis of reaction schemes where equilibria give algebraic constraints on the concentrations.

We define the (n,m) matrix $\underline{W}(t)$ of sensitivity functions as

$$\underline{W}(t) := \frac{\partial \underline{u}(t)}{\partial \underline{\theta}} \tag{3}$$

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This matrix satisfies a set of differential/algebraic equations which can be derived by partial differentiation of equations (1a), (1b) with respect to the parameter vector $\underset{\sim}{\theta}$:

$$\underset{\sim}{E}\underset{\sim}{W}'(t) - \underset{\sim}{J}(t)\underset{\sim}{W}(t) = \frac{\partial}{\partial \underset{\sim}{\theta}} \underset{\sim}{f}(t,\underset{\sim}{u}(t);\underset{\sim}{\theta}) \tag{4a}$$

$$\underset{\sim}{W}(t=t_0) = \frac{\partial \underset{\sim}{u}_0(\underset{\sim}{\theta})}{\partial \underset{\sim}{\theta}} \tag{4b}$$

where the matrix $\underset{\sim}{J}(t)$ (shorthand for $\underset{\sim}{J}(t,u(t);\underset{\sim}{\theta})$) is defined as

$$\underset{\sim}{J}(t) := \frac{\partial}{\partial \underset{\sim}{u}} \underset{\sim}{f}(t,\underset{\sim}{u}(t);\underset{\sim}{\theta}) \tag{5}$$

Various properties of equations (4a) and (4b) are described in Tomovic and Vukobratovic [18]. The most striking feature of these sensitivity equations is that they are linear, regardless of the linearity or nonlinearity of the state equations (1a) and (1b). The problem studied here is the numerical computation of the matrix $\underset{\sim}{W}(t)$ from equations (4a) and (4b).

LITERATURE REVIEW AND THEORETICAL BACKGROUND

Before describing the new algorithm, we review a few known facts about the solution of mixed systems of ordinary differential and algebraic equations. Several investigators [6], [7], [15], have considered this subject and recently Petzold [11] has published an algorithm called DASSL for the solution of such systems.

Not all systems of differential/algebraic equations are solvable. The reader is encouraged to consult the literature, Petzold and Gear [12], and Campbell and Petzold [2], on this peculiar feature of mixed systems. However, for the systems that we are considering, where the matrix

$\underset{\sim}{E}$ assumes the form (2), sufficient conditions are known [12] for the solvability of (1a) and (1b).

Let the function $\underset{\sim}{f}(t,\underset{\sim}{u}(t);\underset{\sim}{\theta})$ be continuously differentiable with respect to $\underset{\sim}{u}(t)$. Now consider the Jacobian matrix $\underset{\sim}{J}(t)$ defined by equation (5) for the system (1a). If we partition the Jacobian matrix according to the partition of $\underset{\sim}{E}$, i.e.,

$$\underset{\sim}{J}(t) = \left[\begin{array}{c:c} \underset{\sim}{J}_{11}(t) & \underset{\sim}{J}_{12}(t) \\ \hdashline \underset{\sim}{J}_{21}(t) & \underset{\sim}{J}_{22}(t) \end{array}\right] \tag{6}$$

where $\underset{\sim}{J}_{11}(t)$ is an (s,s) matrix, then the system (1a) and (1b) is solvable if

$$\det \underset{\sim}{J}_{22}(t) \neq 0 \quad \text{for all} \quad t \tag{7}$$

Under this condition, the solution obtained by a k-step backward differentiation formula algorithm with $k < 7$ and fixed step size h converges to $O(h^k)$ if all initial values are correct. Further aspects of equations (1a) and (1b) and their numerical treatment are discussed in Petzold [13].

Let us now review some of the methods used for the computation of the sensitivity matrix $\underset{\sim}{W}(t)$. With one exception (Stewart and Sørensen [16]) the known methods are for systems of ODE's only; that is, for systems with $\underset{\sim}{E} = \underset{\sim}{I}^{(n)}$. The available algorithms include the Fourier amplitude test [4], direct differential methods [5], Green's function methods [8], the analytically integrated Magnus method [14] (a modification of the Green's function method), and finite difference methods. The Green's function

method and its variations exploit the fact that the sensitivity equations are linear inhomogeneous with time varying coefficients; consequently they can be solved by first calculating the solution of the homogeneous part and then determining the particular solution corresponding to each parameter.

Several authors have proposed to solve the sensitivity equations by extending known solution algorithms for the state equations. This idea is based on the identity of the coefficient matrices in the sensitivity equations to those in the locally linearized form of the state equations on the locus $\underset{\sim}{y}(t)$. Stewart and Sørensen [16], Vemuri and Raefsky [19], Lojek [10], and Hwang [9] have developed various aspects of this method; nevertheless the idea is still under development.

In the present work, we exploit fully the similarity of the sensitivity and state equations, by building the sensitivity analysis into a robust differential/algebraic equation solver. Then we illustrate the algorithm by solving a stiff industrial kinetics problem.

MATHEMATICAL DEVELOPMENT OF THE SENSITIVITY ANALYSIS ALGORITHM

One of the most important steps in developing the sensitivity analysis algorithm was the selection of the integrator. For mixed systems of differential and algebraic equations, there are several codes [7], [11], [15] designed to perform the integration. These codes are primarily based on an idea developed by Gear [6]; specifically, the derivative $\underset{\sim}{y}'(t_{n+1})$ is approximated by a backward difference formula with adaptable order and step size, and the resulting system of nonlinear equations is solved for $\underset{\sim}{y}(t_{n+1})$ via a modified Newton scheme.

We chose for this work the package DASSL developed by Petzold [11].

This package is portable, robust and easy to use. We tested the code successfully on a wide variety of stiff problems, both differential and mixed, before adding the sensitivity analysis algorithm.

First, consider the solution of state and sensitivity equations (1a), (1b), (4a), (4b) as a single system. In this approach, one needs the Jacobian matrix of the total system (1a) and (4a). If we partition the sensitivity matrix $\underline{W}(t)$ into column vectors as

$$\underline{W}(t) = [\underline{w}_1(t) | \underline{w}_2(t) | \cdots | \underline{w}_m(t)] \tag{8}$$

where

$$\underline{w}_i(t) := \frac{\partial \underline{y}(t)}{\partial \theta_i} \qquad i = 1,2, \cdots \ m, \tag{9}$$

then the Jacobian matrix $\underline{J}^*(t)$ (shorthand for $\underline{J}^*(t,\underline{u}(t),\underline{W}(t);\underline{\theta})$) of the total system (1a) and (4a) is

$$\underline{J}^*(t) = \begin{bmatrix} \underline{J}(t) & \underline{0} & \underline{0} & \cdots & \underline{0} \\ \underline{j}_1(t) & \underline{J}(t) & \underline{0} & \cdots & \underline{0} \\ \underline{j}_2(t) & \underline{0} & \underline{J}(t) & & \underline{0} \\ \vdots & \vdots & \vdots & & \vdots \\ \underline{j}_m(t) & \underline{0} & \underline{0} & \cdots & \underline{J}(t) \end{bmatrix} \tag{10}$$

where

$$\underline{j}_i(t) := \frac{\partial \underline{J}(t)}{\partial \underline{y}(t)} \underline{w}_i(t) + \frac{\partial \underline{J}(t)}{\partial \theta_i} \qquad i = 1,2, \cdots m \tag{11}$$

The evaluation of $\underset{\sim}{J}^*(t)$ is a formidable calculation, though a natural requirement of Newton iteration on the total equation system, (1a) and (4a). A simpler and quicker approach is to solve (1a) before (4a) at each time step, as shown below; then the matrices $\underset{\sim}{J}_i(t)$ are not required.

Let $\tilde{\underset{\sim}{u}}^{(r)}(t)$ be the local interpolant of $\underset{\sim}{u}(t)$ obtained in r Newton iterations of a kth-order integrator within a given time step. Then the next iteration will give the interpolant $\tilde{\underset{\sim}{u}}^{(r)}(t) + \Delta\tilde{\underset{\sim}{u}}^{(r)}(t)$, which satisfies the following linearized form of equation (1a)

$$\underset{\sim}{E}(\tilde{\underset{\sim}{u}}'^{(r)}(t)+\Delta\tilde{\underset{\sim}{u}}'^{(r)}(t)) = \underset{\sim}{f}(t,\tilde{\underset{\sim}{u}}^{(r)}(t);\underset{\sim}{\theta})+\underset{\sim}{J}(t,\tilde{\underset{\sim}{u}}^{(r)}(t);\underset{\sim}{\theta})\Delta\tilde{\underset{\sim}{u}}^{(r)} + O(h^k) \quad (12)$$

Hence the correction $\Delta\tilde{\underset{\sim}{u}}^{(r)}$ satisfies

$$\underset{\sim}{E}\Delta\tilde{\underset{\sim}{u}}'^{(r)}-\underset{\sim}{J}^{(r)}(t)\Delta\tilde{\underset{\sim}{u}}^{(r)} = \underset{\sim}{f}(t,\tilde{\underset{\sim}{u}}^{(r)}(t);\underset{\sim}{\theta}) - \underset{\sim}{E}\tilde{\underset{\sim}{u}}'^{(r)}(t) + O(h^k) \quad (13)$$

when the standard Newton method (with $\underset{\sim}{J}^{(r)}(t)$ updated for each iteration) is used. If $\Delta\tilde{\underset{\sim}{u}}^{(r)}(t)$ converges toward zero with increasing r, then $\underset{\sim}{J}^{(r)}(t)$ converges toward $\underset{\sim}{J}(t)$, and equation (13) becomes formally similar to equation (4a). Therefore, we can defer consideration of equation (4a) until $\tilde{\underset{\sim}{u}}^{(r)}(t)$ has converged to $\tilde{\underset{\sim}{u}}(t)$ at the current value of t. Then we can update the sensitivity solution $\tilde{\underset{\sim}{W}}(t)$ directly by use of equation (4a), which has the same coefficients as equation (13) but a different, now computable right hand function. More specifically the corrections $\Delta\tilde{\underset{\sim}{w}}_i(t)$ are calculated via a single iteration by solving

$$\underset{\sim}{E}\Delta\tilde{\underset{\sim}{w}}_i'(t)-\underset{\sim}{J}(t)\ \Delta\tilde{\underset{\sim}{w}}_i(t) = -\underset{\sim}{E}\tilde{\underset{\sim}{w}}_i'^{(p)}(t)+\underset{\sim}{J}(t)\ \tilde{\underset{\sim}{w}}_i^{(p)}(t) + \frac{\partial}{\partial\theta_i}\underset{\sim}{f}(t,\tilde{\underset{\sim}{u}}(t);\underset{\sim}{\theta}) + O(h^k)$$

$$i = 1,2, \cdots m \quad (14)$$

in which $\tilde{w}_i^{(p)}(t)$ is the predicted value of $\tilde{w}_i(t)$ via a kth-order predictor formula.

The vectors $\tilde{w}_i(t)$ are calculated at the current t as follows:

$$\tilde{w}_i(t) = \tilde{w}_i^{(p)}(t) + \Delta\tilde{w}_i(t) \qquad i = 1,2, \cdots m \tag{15}$$

On completion of the update, the local truncation error is tested, and if necessary the step size h and approximation order k are adjusted to achieve the specified accuracy for $\underset{\sim}{y}(t)$ and $\underset{\sim}{W}(t)$.

Numerical tests show that stringent tolerances on $\underset{\sim}{y}(t)$ normally lead to a good solution for $\underset{\sim}{W}(t)$ as well, provided that $\underset{\sim}{J}(t)$ is updated before computing $\Delta\tilde{\underset{\sim}{W}}(t)$. On the other hand, if the iteration matrix is only occasionally updated (as is usual in implicit integrators), then the local tolerances on $\underset{\sim}{W}(t)$ are essential to control the calculation.

COMPUTER IMPLEMENTATION

The computer implementation of the sensitivity analysis algorithm was done as follows:

1) The working arrays used by DASSL were modified to provide storage allocation for the sensitivity functions.
2) An algorithm was written for the automatic formation of the sensitivity equations.
3) The integrator in DASSL was properly extended to include the solution of the sensitivities.

The following definitions were adopted:

1) Iteration matrix $\underset{\sim}{D}(t) := c\underset{\sim}{E} - \underset{\sim}{J}(t)$, where c is a constant which depends on step size history

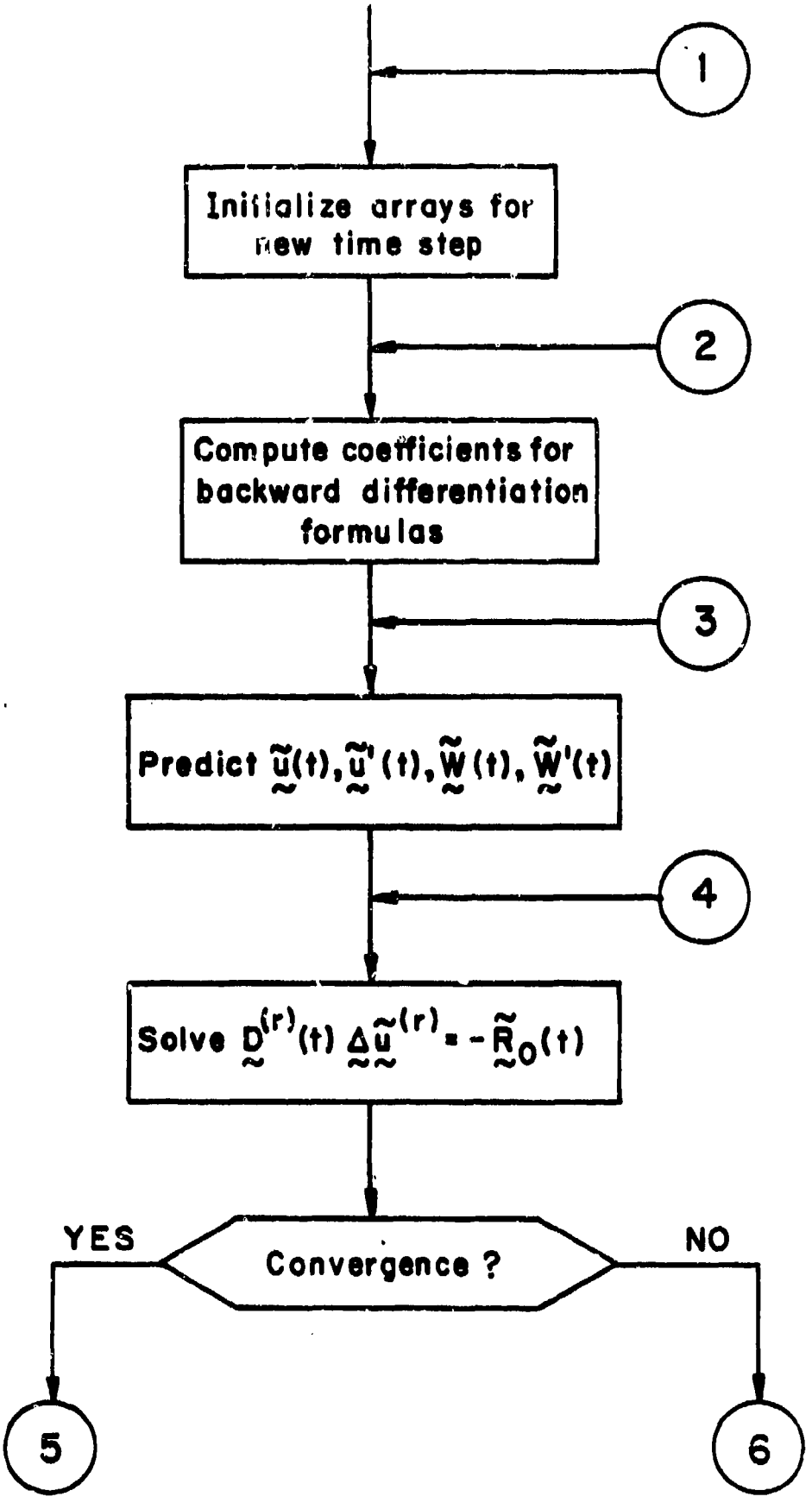
2) Residual of the state equations

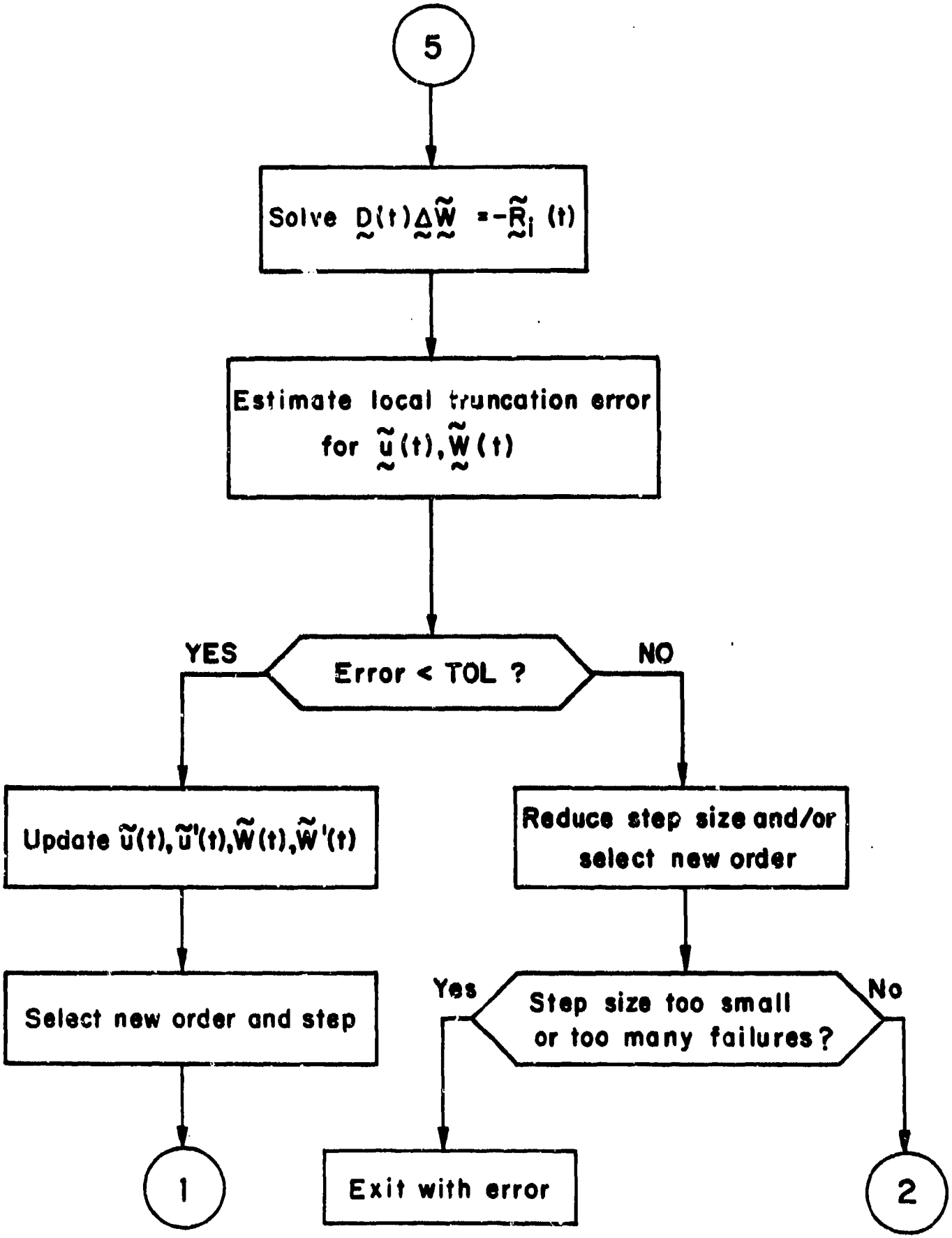
$$\underset{\sim}{R}_0(t) := \underset{\sim}{E}\underset{\sim}{u}'(t) - \underset{\sim}{f}(t,\underset{\sim}{u}(t);\underset{\sim}{\beta})$$

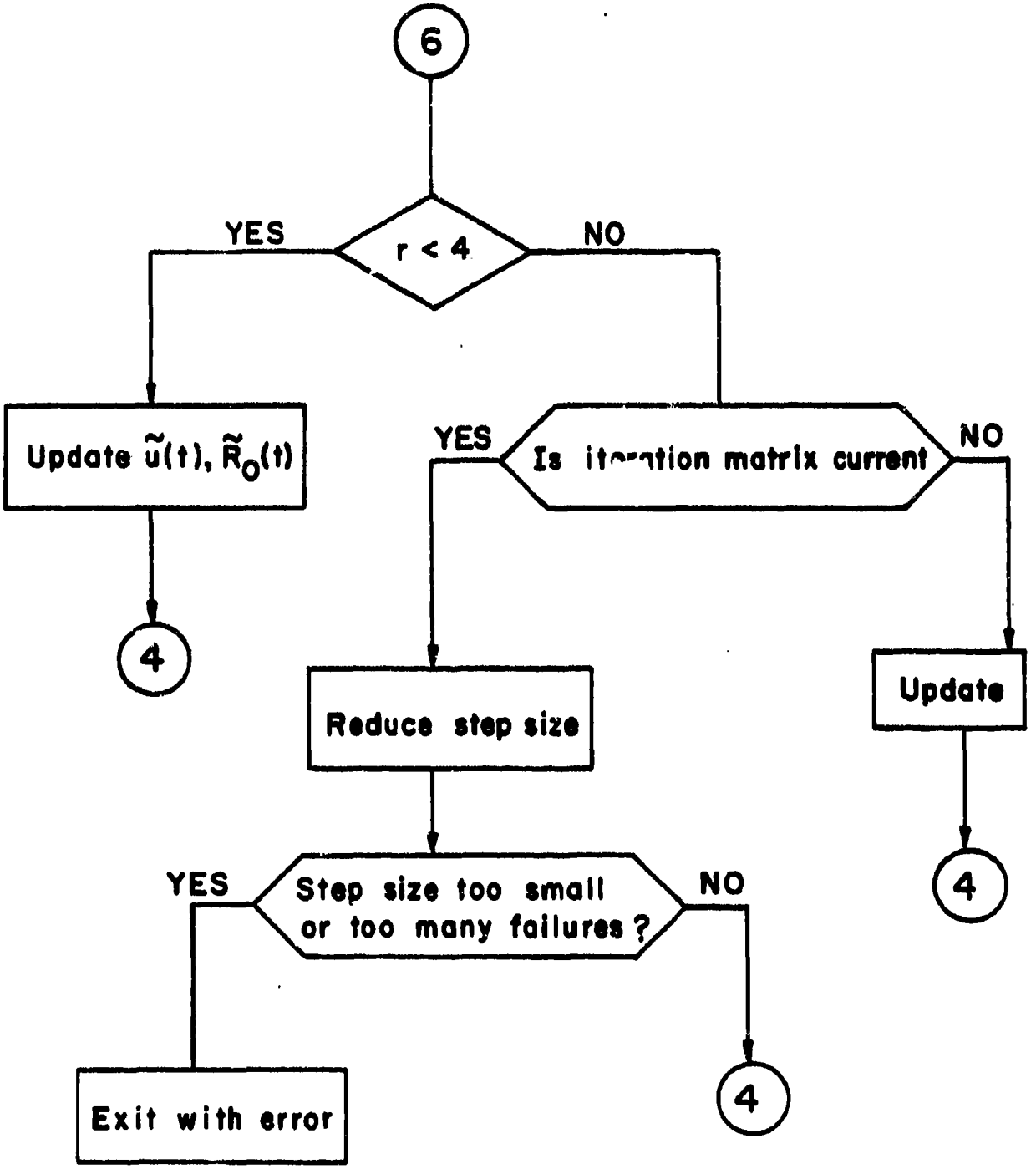
3) Residual of the sensitivity equations

$$\underset{\sim}{R}_i(t) := \underset{\sim}{E}\underset{\sim}{w}_i'(t) - \underset{\sim}{J}(t)\underset{\sim}{w}_i(t) - \frac{\partial}{\partial\theta_i}\underset{\sim}{f}(t,\underset{\sim}{u}(t);\underset{\sim}{\beta}) \qquad i = 1,2, \cdots m$$

The calculation sequence is outlined in the adjoining flow chart.


1
Initialize arrays for new time step
2
Compute coefficients for backward differentiation formulas
3
Predict $\tilde{u}(t), \tilde{u}'(t), \tilde{W}(t), \tilde{W}'(t)$
4
Solve $\tilde{D}^{(r)}(t)\,\Delta\tilde{u}^{(r)} = -\tilde{R}_0(t)$
YES
Convergence ?
NO
5
6


5
Solve $\underset{\sim}{D}(t)\Delta\underset{\sim}{\tilde{W}} = -\underset{\sim}{\tilde{R}}_i(t)$
Estimate local truncation error for $\underset{\sim}{\tilde{u}}(t), \underset{\sim}{\tilde{W}}(t)$
YES
Error < TOL ?
NO
Update $\tilde{u}(t), \tilde{u}'(t), \tilde{W}(t), \tilde{W}'(t)$
Reduce step size and/or select new order
Select new order and step
Yes
Step size too small or too many failures?
No
1
Exit with error
2


6
YES
r < 4
NO
Update $\tilde{u}(t)$, $\tilde{R}_0(t)$
YES
Is iteration matrix current
NO
4
Reduce step size
Update
YES
Step size too small
or too many failures ?
NO
4
Exit with error
4

NUMERICAL EXAMPLE

The algorithm was tested on a wide variety of problems, ranging from linear and nonlinear systems of differential equations to large systems of differential and algebraic equations. We present here a batch reactor example given by the Dow Chemical Company [1]. Figure 1 shows the proposed mechanism for the reaction system. The time dependent concentrations are modelled by the following system of differential and algebraic equations:

$$
\begin{aligned}
u_1'(t) &= -k_2 u_2(t) u_8(t) \\
u_2'(t) &= -k_1 u_2(t) u_6(t) + k_{-1} u_{10}(t) - k_2 u_2(t) u_8(t) \\
u_3'(t) &= k_2 u_2(t) u_8(t) + k_3 u_4(t) u_6(t) - k_{-3} u_9(t) \\
u_4'(t) &= -k_3 u_4(t) u_6(t) + k_{-3} u_9(t) \\
u_5'(t) &= k_1 u_2(t) u_6(t) - k_{-1} u_{10}(t) \\
u_6'(t) &= -k_1 u_2(t) u_6(t) - k_3 u_4(t) u_6(t) + k_{-1} u_{10}(t) + k_{-3} u_9(t) \\
u_7(t) &= -0.0131 + u_6(t) + u_8(t) + u_9(t) + u_{10}(t) \qquad (16) \\
u_8(t) &= \frac{K_2 u_1(t)}{K_2 + u_7(t)} \\
u_9(t) &= \frac{K_3 u_3(t)}{K_3 + u_7(t)} \\
u_{10}(t) &= \frac{K_1 u_5(t)}{K_1 + u_7(t)}
\end{aligned}
$$

Figure 1. Chemical reaction model for the numerical example [1]. The numbers are used for the enumeration of the chemical species. as in equation (16).

Slow Kinetic Reactions

$$^{6}M^{-} + {}^{2}BM \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} {}^{10}MBM^{-}$$

$$^{8}A^{-} + BM \xrightarrow{k_2} {}^{9}ABM^{-}$$

$$M^{-} + {}^{4}AB \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} ABM^{-}$$

Rapid Acid-Base Reactions

$$^{5}MBMH \overset{K_1}{\rightleftharpoons} MBM^{-} + {}^{7}H^{+}$$

$$^{1}HA \overset{K_2}{\rightleftharpoons} A^{-} + H^{+}$$

$$^{3}HABM \overset{K_3}{\rightleftharpoons} ABM^{-} + H^{+}$$

Figure 1.

with initial conditions

$$u_1(0) = 1.5776$$

$$u_2(0) = 8.32$$

$$u_j(0) = 0 \quad j = 3,4,5,9,10 \tag{17}$$

$$u_6(0) = 0.0131$$

$$u_7(0) = 0.5\{-K_2 + \sqrt{K_2^2+4K_2u_1(0)}\}$$

$$u_8(0) = u_7(0)$$

The following values of rate and equilibrium constants were used [3]

$$k_1 = 21.893 \qquad hr^{-1}\ Kg\ gmole^{-1}$$

$$k_{-1} = 2.14\ E09 \qquad hr^{-1}$$

$$k_2 = 32.318 \qquad hr^{-1}\ Kg\ gmole^{-1}$$

$$k_3 = 21.893 \qquad hr^{-1}\ Kg\ gmole^{-1} \tag{18}$$

$$k_{-3} = 1.07\ E09 \qquad hr^{-1}$$

$$K_1 = 7.65\ E-18 \qquad gmole\ Kg^{-1}$$

$$K_2 = 4.03\ E-11 \qquad gmole\ Kg^{-1}$$

$$K_3 = 5.32\ E-18 \qquad gmole\ Kg^{-1}$$

The natural logarithms of these constants make up the parameter vector $\underset{\sim}{\theta}$. Our goal is to estimate the sensitivity matrix $\underset{\sim}{W}(t) = \frac{\partial \underset{\sim}{y}(t)}{\partial \underset{\sim}{\theta}}$.

The combined system of state and sensitivity functions consists of 90 equations, 54 of which are differential and 36 are algebraic. This problem presents a severe test for the DASSL integrator and the sensitivity analysis algorithm.

Table 1. summarizes the computational effort for the solution of the above problem on a VAX 11/780 computer. All calculations were carried out in double precision. A mixed local truncation error control provided in [11] was used. The tolerances for the sensitivities were equated to the tolerances of the state variables. The total reaction time considered was 53 hr.

Figures 2 and 3 show the evolution of the concentration profiles as a function of time, while Figures 4 through 11 show the dynamic behavior of the sensitivity functions.

Sensitivity plots, like those in Figures 4-11, can be of considerable use to the theoretician as well as to the experimentalist. From Figures 4 through 11 we see that all of the rate and equilibrium constants have comparable effects on the concentrations and therefore we cannot eliminate any step from the proposed mechanism in Figure 1. However, a close inspection of the results reveals the following linear relations:

$$k_{-1} \frac{\partial \underset{\sim}{y}(t)}{\partial k_{-1}} = - K_1 \frac{\partial \underset{\sim}{y}(t)}{\partial K_1} \tag{19}$$

$$k_{-3} \frac{\partial \underset{\sim}{y}(t)}{\partial k_{-3}} = K_3 \frac{\partial \underset{\sim}{y}(t)}{\partial K_3} \tag{20}$$

TABLE 1.

Computational effort for the solution of the Dow problem

	STATE EQUATIONS		SENSITIVITY EQUATIONS	
	e*=1.0E-6	e=1.0E-7	e=1.0E-6	e=1.0E-7
Time steps :	191	265	187	264
Function evaluations:	418	587	383	534
CPU secs :	4.0	5.5	23.5	33

* local error test at each time step which requires roughly that abs (local error) less or equal than rtol•abs(u)+atol where rtol=atol=e.

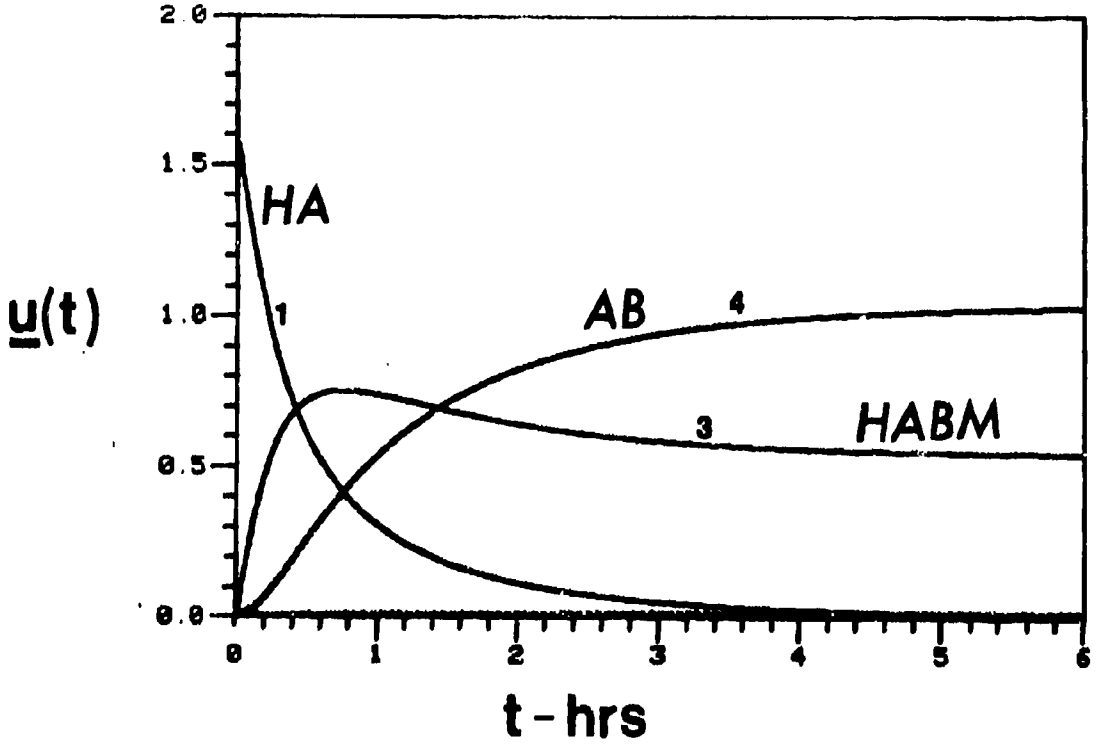


Figure 2.

Figure 2. Concentration functions $u_i(t)$ in gmole/kg.

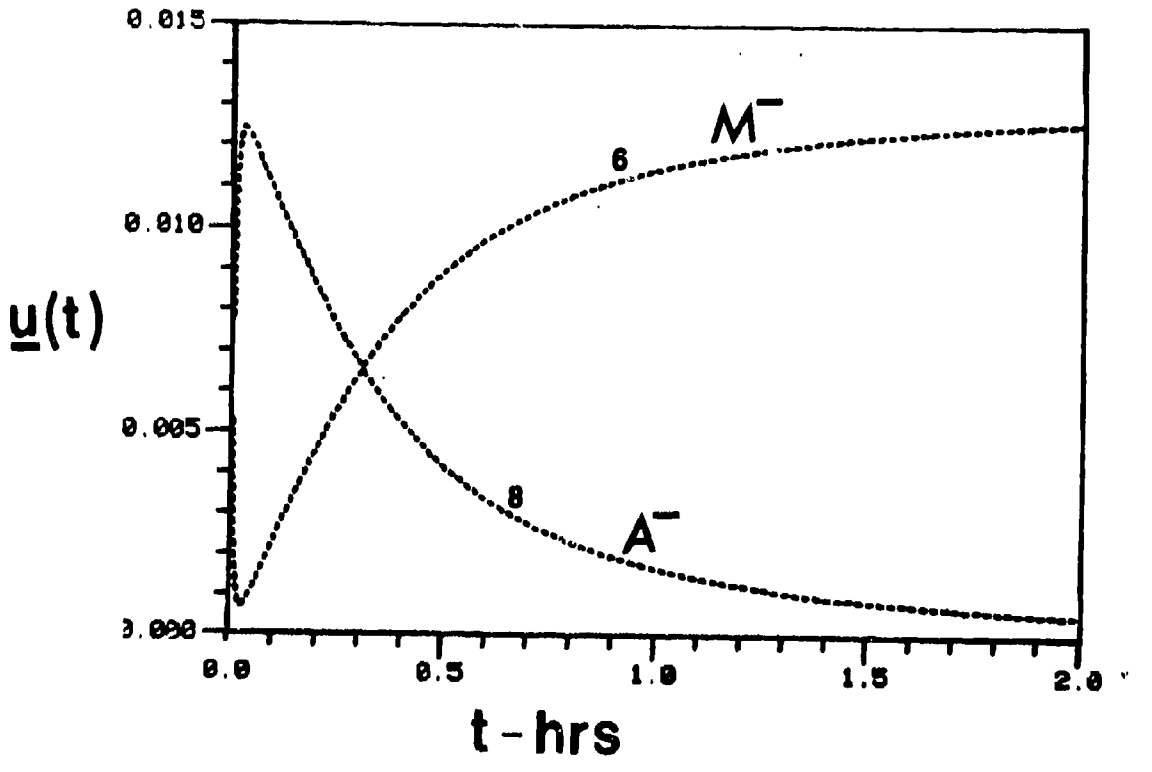


Figure 3.

Figure 3. Concentration functions $u_i(t)$ in gmole/kg.

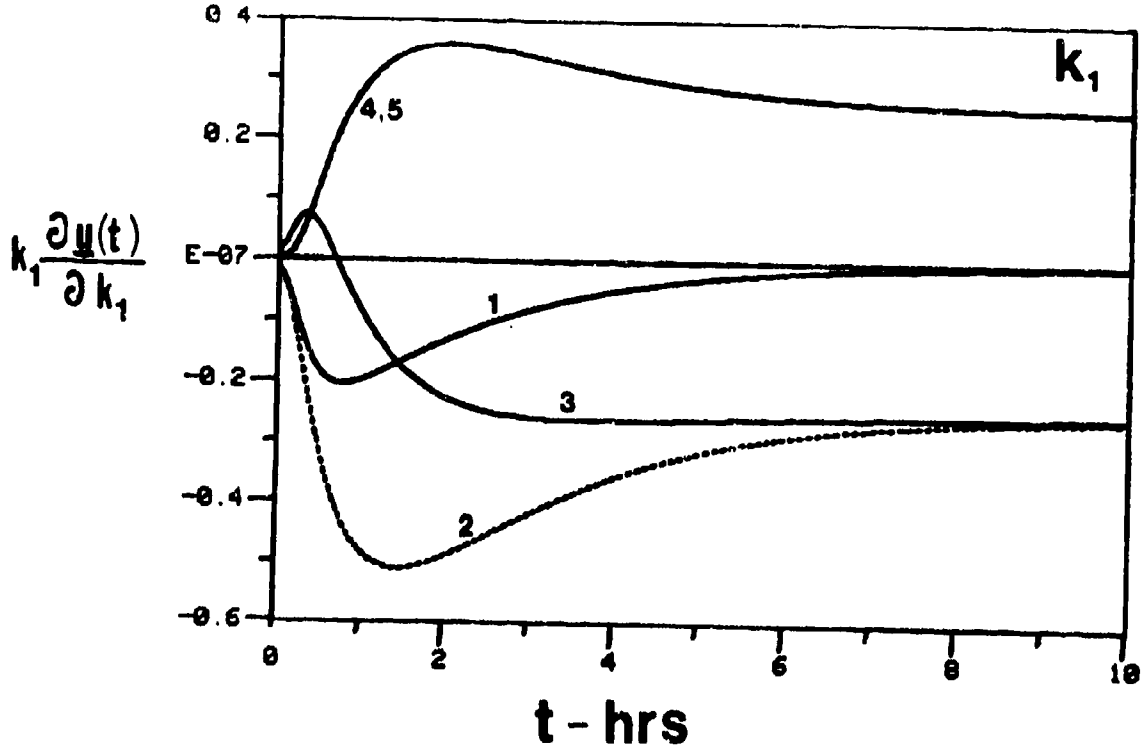


Figure 4.

Figure 4. Elements of the sensitivity vector $\frac{\partial \underline{u}(t)}{\partial \ell n k_1}$. The number ℓ denotes the sensitivity coefficient $u_\ell(t)$ with respect to $\ell n k_1$. Numbers not shown correspond to sensitivity functions indistinguishable from zero at all times.

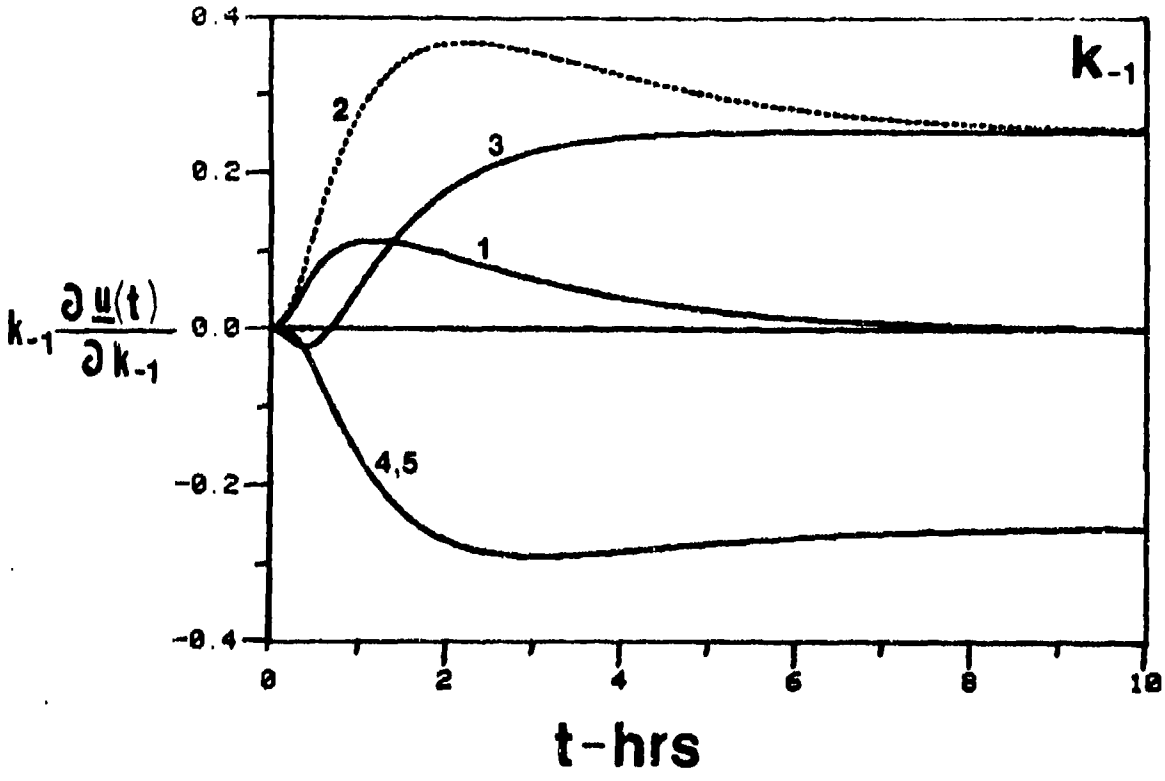


Figure 5.

Figure 5. Elements of the sensitivity vector $\partial \underline{y}(t)/\partial \ell n k_{-1}$.

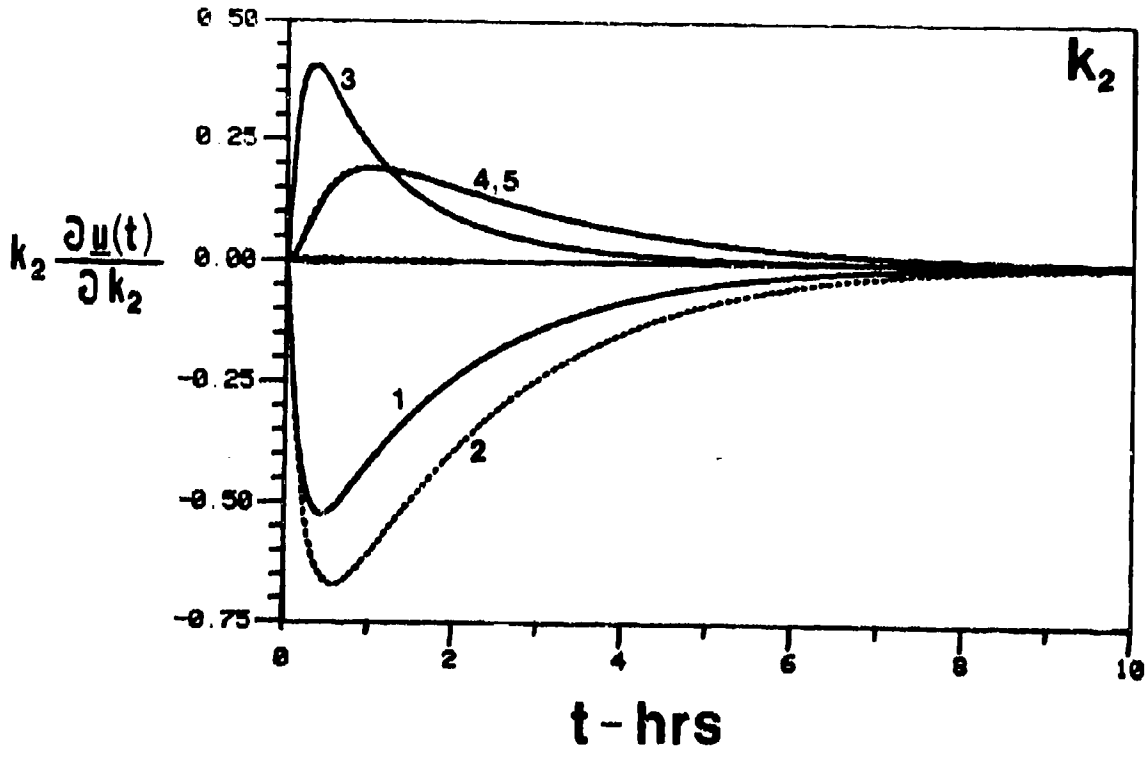


Figure 6.

Figure 6. Elements of the sensitivity vector $\partial \underline{y}(t)/\partial \ell n k_2$.

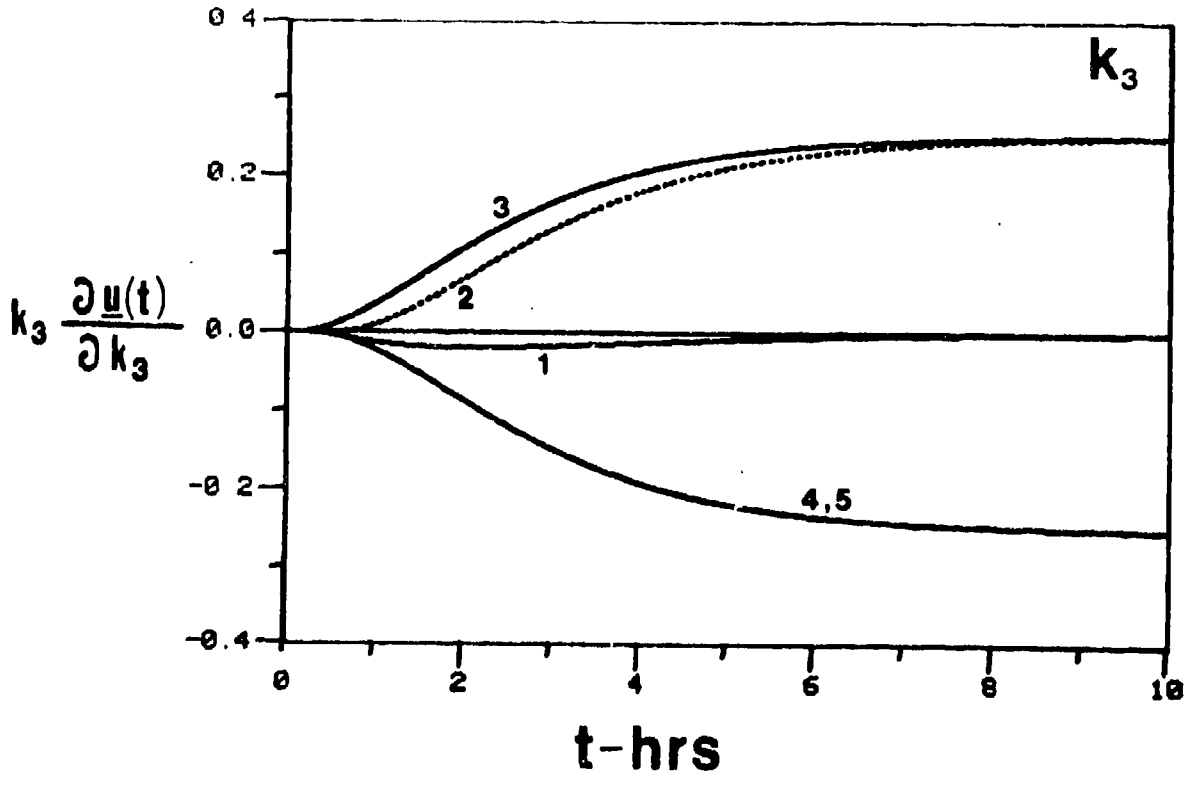


Figure 7.

Figure 7. Elements of the sensitivity vector $\partial \underline{y}(t)/\partial \ell n k_3$.

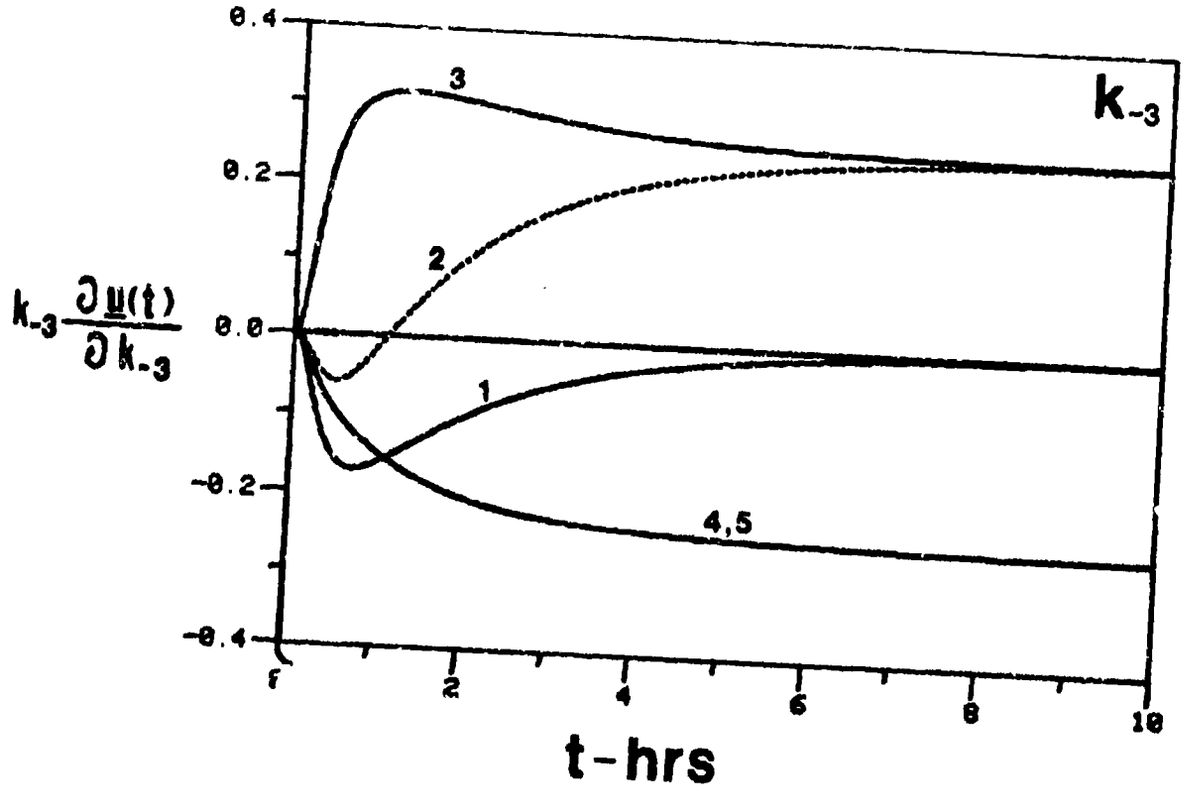


Figure 8.

Figure 8. Elements of the sensitivity vector $\partial \underline{y}(t)/\partial \ell nk_{-3}$.

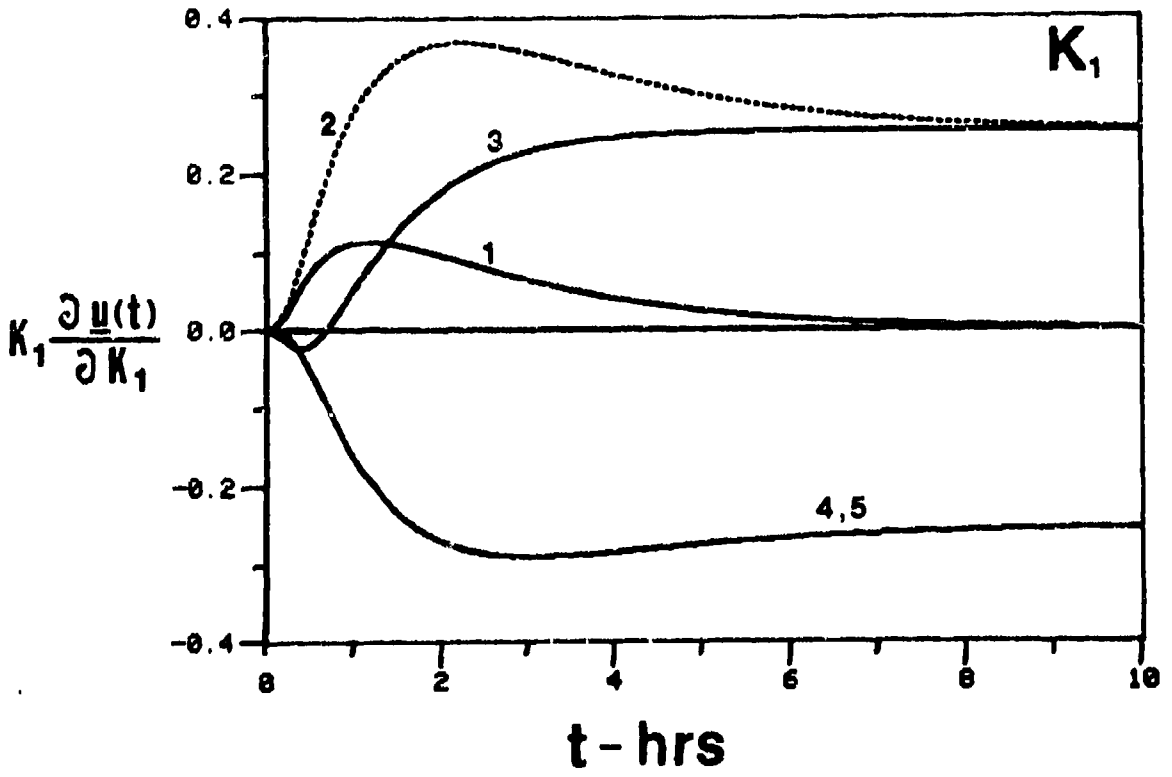


Figure 9.

Figure 9. Elements of the sensitivity vector $\partial \underset{\sim}{u}(t)/\partial \ell n k_1$.

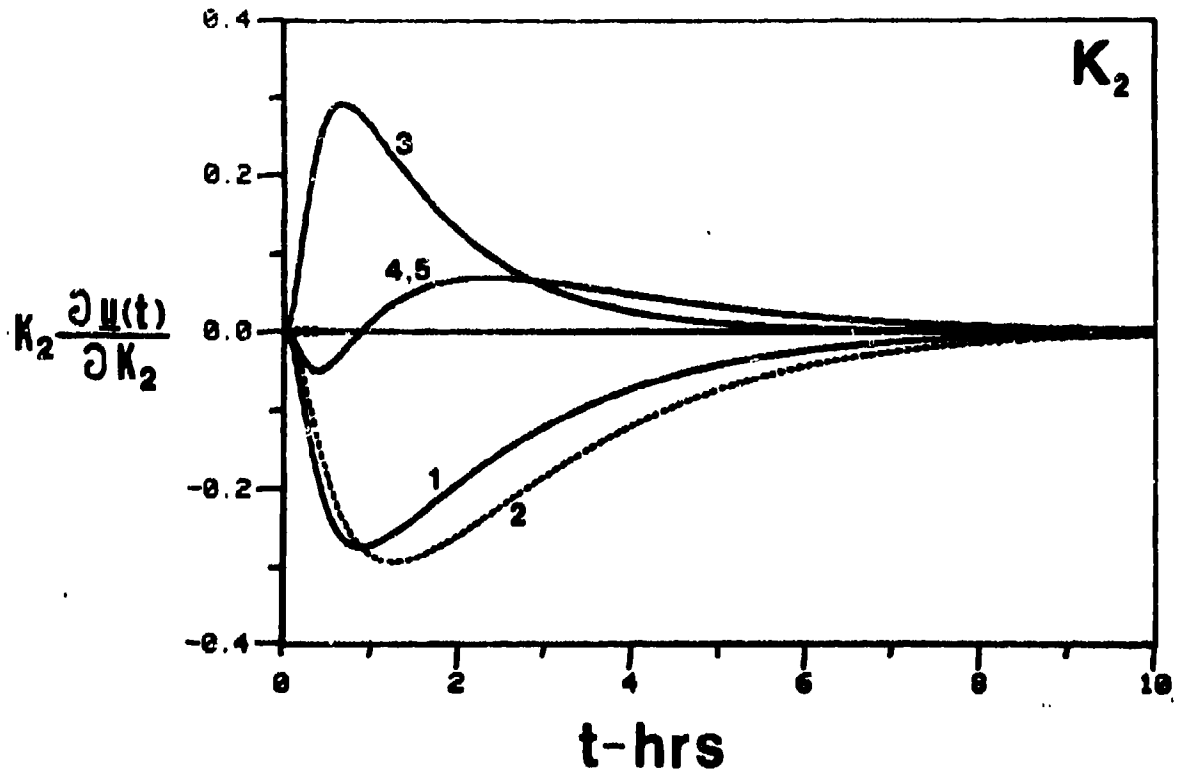


Figure 10.

Figure 10. Elements of the sensitivity vector $\partial \underline{y}(t)/\partial \ell n k_2$.

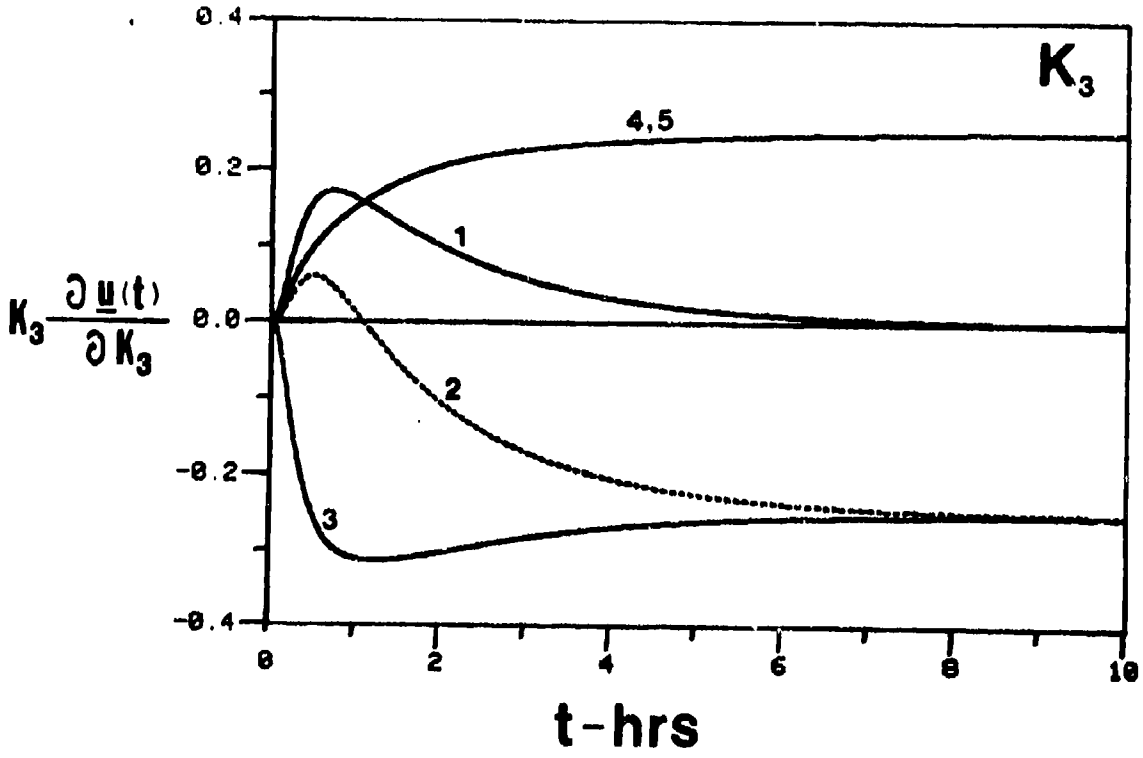


Figure 11.

Figure 11. Elements of the sensitivity vector $\partial \underset{\sim}{u}(t)/\partial \ell n k_3$.

Thus, one cannot estimate all parameters of the model from data on $\underline{y}(t)$. Equations (19) and (20) indicate that (k_{-1}/K_1) and $k_{-3}K_3$ should be used as parameters; then the predicted $\underline{y}(t)$ is invariant to K_1 and K_3. This information proved useful in fitting the model (16), (17) to the published experimental data for this system [3].

CONCLUSIONS AND SIGNIFICANCE

An efficient method has been developed here for the calculation of parametric sensitivities for mixed systems of ordinary differential and algebraic equations. The method has been tested successfully on many problems, ranging from simple ODE's to large stiff systems of differential and algebraic equations. The scheme has been implemented for a robust implicit integrator (DASSL), and is applicable to any implicit integrator.

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An efficient method is described for sensitivity analysis of nonlinear initial value problems, which may include algebraic equations as well as ordinary differential equations (ODE's).

The linearity of the sensitivity equations is utilized to solve them directly via the local Jacobian of the state equations. The method is implemented with the implicit integrator DASSL and is demonstrated on a stiff industrial reaction model.

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